Augmented partial factorization: efficient computation of the generalized scattering matrix

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Abstract

Simulations of PDEs typically involve computing the solution on every element of a large discretization basis set, but oftentimes the quantities of interests are contained in a much smaller number of projections (described by the rows of a fat output-projection matrix C). When multiple right-hand sides are of interest (given by the columns of a tall input-source matrix B), a loop is typically used to go over the right-hand sides during the solution phase, which becomes the speed bottleneck when the number of right-hand sides is large. Furthermore, storage of the LU factors uses significant memory and/or disk space. Problems of this type are very common, and they require computing C*inv(A)*B, which is a generalized scattering matrix. We propose to compute C*inv(A)*B by first building an augmented sparse matrix K = [A, B; C, 0] and then using MUMPS to obtain its Schur complement. Doing so only uses a single partial factorization, without a solution phase, without storing the LU factors, and without solving the PDE on every element of its discretization basis set. We apply this "augmented partial factorization" approach to the simulation of multi-channel optical systems governed by Maxwell's equations and realize over three-orders-of-magnitude speed-up as well as memory usage reduction.

Reference: Ho-Chun Lin, Zeyu Wang, and Chia Wei Hsu, Fast multi-source nanophotonic simulations using augmented partial factorization, Nature Computational Science 2, 815 (2022).